MASLOV, P. G.

USSR/Physics - Atomic Forces
Mathematics - Matrices

PA 165T66

21 Feb 50

"Determination of the Inverse Matrices of Potential Energy of Polyatomic Molecules (Approximation Methods for Finding the Coefficients of Influence)," P. G. Maslov, Leningrad Mil Mech Inst

"Dok Ak Nauk SSSR" Vol LXX, No 6, pp 985-988

Elements of inverse potential-energy matrices, namely coefficients K_{ij}^* of influence, possess valuable advantage over dynamic coefficients and so-called quasi-elastic constants, when one attempts unique description

USSR/Physics - Atomic Forces
(Contd)

21 Feb 50

165T66

of interaction of forces in a molecule, since dynamic coefficients are noninvariant to transformations of coordinates. Submitted 24 Dec 49 by Acad V. A. Fok,

Calculation of reciprocal matrices of the potential energy of polyatomic molecules (the method of combined steepest descent). P. G. Maslov (Leningrad Military Mechanic Inst.). *Doklady Akad. Nauk S.S.S.R.* **71**, 867–70(1950); cf. *C.A.* **44**, 5308i.—Theoretical. The action coeffs. of the generalized forces in the potential-energy matrix of polyatomic mols. can be calcd. without knowing the dynamic consts. and without making the tedious transformation from the matrix of dynamic coeffs. to the matrix of the kinetic energy. Approx. values of the action coeffs. are obtained by solving the general equations of vibrating atoms ($GX - A)Q = 0$ where G is the unknown matrix of the action coeffs., A is the matrix of kinetic coeffs., Q is the vector component of generalized force Q_i, and A is the square of the vibration frequency. Comparison of the calcd. frequencies with the observed permits estn. of the effect of the individual action coeffs. on the calcd. frequencies. The calcn. is shortened considerably by using a method of combined steepest descent for the soln. of the general equations. The method is described and illustrated in detail. In practice, only one cycle of descent need be calcd., whereas the integration method and the method of steepest descent may require 3 or 4 successive approximations.   M. J. Sienko

MASLOV, P. G.

USSR/Chemistry - Methane, Ethane   May 51

"Concerning Determination of Coefficients of Influ-
ence for Oscillations of Polyatomic Molecules. I.
Coefficients of Influence of Methane, Deuteromethane;
Ethane, and Deuteroethanes," P. G. Maslov, S. A. Anti-
pina, Leningrad

"Zhur Fiz Khim" Vol XXV, No 5, pp 594-605

Calcd coeff's of influence of methane, deuteromethanes,
ethane, and deuteroethane C_2D_6. Established that the
interactions between coordinates are weak; use of
proximate method of detn is preferable. Replacement
in CH_4 of one H with CH_3 does not affect substantially

LC   190T13

USSR/Chemistry - Methane, Ethane (Contd)   May 51

the electronic configuration of the remaining portion
of the CH_4 mol. Reduction of strength of C-H (1)
bonds in such conversion is not ~3%, as it follows
from B. I. Stepanov's work, but approx 1.6%.

LC   190T13

MASLOV, P. G.

134

THE DETERMINATION OF THE EFFECTIVE COEFFICIENTS OF THE VIBRATIONS OF POLYATOMIC MOLECULES. 2. THE POTENTIAL ENERGY CONSTANTS OF HALOGEN SUBSTITUTED METHANE. P. G. Maslov. Translated by Esther Rabkin from Zhur. Fiz. Khim. 25, 803-13 (1951). 22p (TT-301)

The effective coefficients of the halogen methanes CH_3X, CH_2X_2, CHX_3, CX_4, (X = Br, Cl, F) were obtained by the method of determinants. By the method of the combined fastest emission the effective coefficients of the iodo-substituted methanes were obtained; also, a calculation and an interpretation of the frequencies of these molecules were carried out. An error was discovered in the interpretation of the frequencies of the molecule CH_2I_2 carried out by Ta-You-WU: the frequencies 1350, 1130, 1027, and 713 cm^{-1} assigned by Ta-You-WU to the vibrations of the type $B_2(\delta)$, $A_1(a\delta)$, $B_1(\delta)$ and $A_2(\delta)$ should be assigned to the vibrations $A_1(a\delta)$ $B_2(\delta)$, $A_2(\delta)$ and $B_1(\delta)$. It was shown that it is inadmissible to carry out a calculation of the frequencies of molecules by neglecting the nondiagonal effective coefficien If the super halogen, F, is excluded, then the transitions $CH_4 \rightarrow CI_4$, $CH_4 \rightarrow CBr_4$, and $CH_4 \rightarrow CCl_4$ for all types of molecules practically do not change the strength of the bond C - H and C - X. The transition $CH_4 \rightarrow CF_4$ increases

the strength of the bond C-F by approximately 20% and
decreases the strength of the bond C-H. (auth)

MASLOV, P. G.

USSR/Chemistry - Organic and Inorganic   Jul 51
                  Halogen Compounds

"Determination of Influence Coefficients for Vi-
brations of Polyatomic Molecules, III. Relation
of Influence Coefficients to Other Molecular Para-
meters," P. G. Maslov, Leningrad

"Zhur Fiz Khim" Vol XXV, No 7, pp 814-822

Established that influence coeffs have advantages
over widely used dynamic consts. Influence co-
effs should therefore be detd at least along with
dynamic consts. Established empirically rela-
tionships of influence coeffs of halogen-substi-
tuted methanes, H, Na, and K halides (for I, Br,

USSR/Chemistry - Organic and Inorganic   Jul 51
                  Halogen Compounds (Contd)

Cl, F) to bond polarizability, equil bond lengths,
and affinity of halogen atoms to electrons in these
compds. Detn of influence coeffs by expt may allow
possibility of detg these parameters accurately
from graphs, which conclusion might conceivably be
extended to crystals.

MASLOV, P. G.

USSR/Physics - Kinetic Theory   11 Aug 51
              of Molecules

"Supplementary Condition Between the Coordinates of
a Central-Force System and the Rules of Its Compu-
tation in Equations and Matrices," P.G. Maslov

"Dok Ak Nauk SSSR" Vol LXXIX, No 5, pp 767-770

Gives the form of the supplementary condition in
connection with an n-atom branched mol described
in a valent-force system. Derives the rule for
calcg the supplementary relations between coordi-
nates of a central-force system in eqs of motion.
Submitted by Acad V.A. Fok 15 Jun 51.

210T85

USSR/Nuclear Physics - Molecular Spectra   Feb 52

"Application of Influence Coefficients to Study of Oscillatory Spectra of Multiatomic Molecules. I. Formula to Find Force Distribution According to Molecular Bonds; Forms of Oscillations; and Interaction of Frequencies in Molecular Oscillations. II. Influence Coefficients; Frequencies, Oscillation Forms Force Distribution, and Analysis of Interaction Character of Frequencies in Acetylene and Deutero-Acetylenes," P.G. Maslov, S.A. Antipina, Leningrad

"Zhur Eksper i Teoret Fiz" Vol XXII, No 2, pp 164-183

USSR/Nuclear Physics - Molecular Spectra   Feb 52
(Contd)

I. Derives formulas. II. System of influence coeff of acetylene is computed, and spectrum of basic frequencies, force distribution with respect to bonds, and oscillation forms is derived. Indebted to Prof M.A. Yel'yashevich. Received 3 Apr 51.

MASLOV, P. G.

MASLOV, P. O.

TT.366 (A method for the solution of a system of homogeneous equations in the calculation of the vibrations of polyatomic molecules) Metod resheniia odnorodnykh lineinykh uravnenii pri raschete kolebanii mnogoatomnykh molekul.
Zhurnal Eksperimental'noi i Teoreticheskoi Fiziki, 22(3): 276-283, 1952.

USSR/Mathematics - Oscillations, Molecules   Mar 52

"Method of Solving a System of Homogeneous Linear
Equations During Computation of Oscillations of
Polyatomic Molecules," P. G. Maslov, Leningrad

"Zhur Eksper i Teoret Fiz" Vol XXII, No 3, pp 276-283

The method of solving eqs of the type $(G) \lambda - A) r = 0$
allows one to det not only the roots lambda and
proper (eigen) vectors r, but also the sensitivity
of frequencies and proper vectors to variations of
parameters and therefore expansion of frequencies

215T43

into parts due to this or another parameter. In-
debted to Prof M. A. Iel'yashevich. Received
19 Apr 51.

215T43

MASLOV, P.G.

USSR/Physics - Molecular Spectra, Deuterium   Jun 52

"Oscillation Spectra and Coefficients of Influence of Ethane and Deuteroethane Molecules," S. A. Antipine, P. G. Maslov, Leningrad

"Zhur Eksper i Teoret Fiz" Vol XXII, No 6, pp 705-715

Obtains a more accurate system of the potential-energy consts $K*_{ij}$ of ethane C_2H_6 and deuteroethane C_2D_6 independently of the familiar system of these mols (B. I. Stepanov, dynamic coeffs of

"Zhur Fiz Khim" 15, 865, 1941). Obtains 1st derivs of frequencies with respect to the parameters k_{ij}, and expands the oscillation frequencies into terms each of which depends only on a definite parameter. Indebted to Prof M. A. Yel'yashev. Received 11 Jul 51.

217T95

MASLOV, P. G.

MASLOV, P. G.

USSR/Physics - Oscillation Spectra   Jun 52

"Oscillation Spectra of Dimethylacetylene," P. G. Maslov, Leningrad

"Zhur Eksper i Teoret Fiz" Vol XXII, No 6, pp 716-727

Computes the oscillation frequencies of the dimethylacetylene mol using coeffs of influence of ethane and acetylene. Interprets spectra of oscillation frequencies of this mol. Finds the sensitivity of frequencies, decomposes the ground frequencies into parts due to parameters $k*_{ij}$ and a_{ij} of the mol. Indebted to Prof M. A. Yel'yashev. Received 11 Jul 51.

217496
217706

Maslov, P. G.

USSR.

539.132

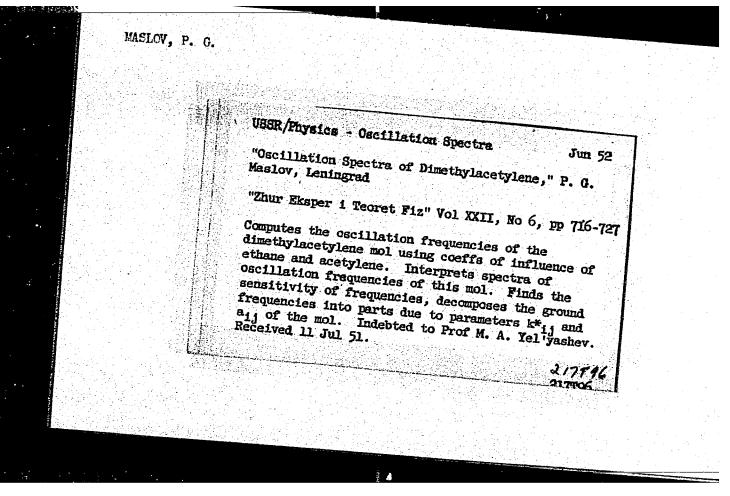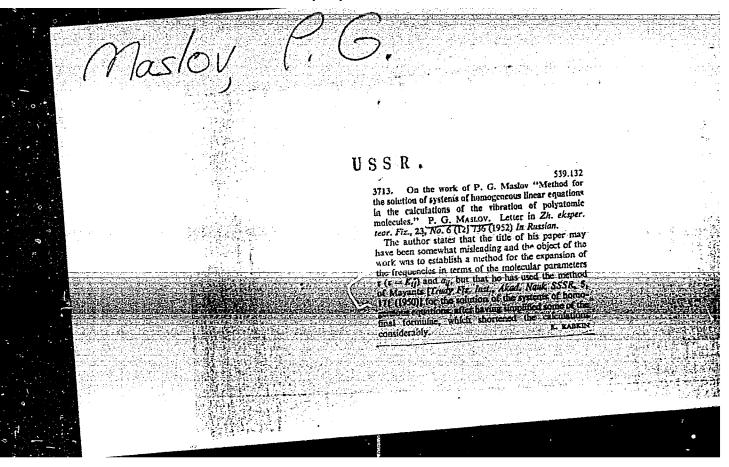3713. On the work of P. G. Maslov "Method for the solution of systems of homogeneous linear equations in the calculations of the vibration of polyatomic molecules." P. G. MASLOV. Letter in *Zh. eksper. teor. Fiz.*, 23, No. 6 (12) 736 (1952) *In Russian.*

The author states that the title of his paper may have been somewhat misleading and the object of the work was to establish a method for the expansion of the frequencies in terms of the molecular parameters $(\varepsilon = \kappa_{ij})$ and a_{ij}, but that he has used the method of Mayants [*Trudy Fiz. Inst. Akad. Nauk SSSR*, 5, 178 (1950)] for the solution of the systems of homogeneous equations after having simplified some of the final formulae, which shortened the calculations considerably.

E. RABKIN

MASLOV, P. G.

Thermodynamics of individual hydrocarbons. I. Calculation of thermodynamic functions of molecules by means of parameters. P. G. Maslov. Zhur. Fiz. Khim. 26, 1311–25(1952); cf. Zhur. Ekspd. i. Teoret. Fiz. 22, 705(1952); following abstrs.—Thermodynamic functions of ethane (I) were detd. from the mol. parameters (coeffs. of influence and kinematic coeffs.). Owing to mol. interactions, the principle of additivity of bond energies does not hold. The wave-no. for torsional vibration of the CH_3 group in I is 243 cm.$^{-1}$ The C-C and C-H bond energies in I are 23 and 56 kcal./mol., resp.; the corresponding electronic energies are 24 and 59 kcal./mol. The heat of combustion $W°$, the heat of formation $E°$, and the electronic energy $E_e°$ in kcal./mol. for normal alkanes in the gas phase at 298.16°K. and 1 atm. can be calcd. by means of the equations $W° = (372.8 + 157.44028(n - 2))$, $E° = (575.8 + 234(n - 2))$, and $E_e° = (616.6 + 248.0(n - 2))$, where n is the no. of C atoms in the mol. Calcd. values of $E°$ and $E_e°$ agree with expt. within 2% for CH_4 and within 0.6% for other alkanes. Tables are given of the distribution of null vibrational energy, free energy, entropy, $W°$, $E°$, and $E_e°$ for normal vibrations of I among bonds, angles, and interactions, as well as vibrational energies of normal alkanes from CH_4 to C_nH_{2n} at 298.10°K.   J. W. Loweberg, Jr.

MASLOV, P. G.

USSR/Chemistry - Hydrocarbons   11 Jun 52

"The Thermodynamics of Individual Hydrocarbons,"
P. G. Maslov, Leningrad Mil Mech Inst

"Dok Ak Nauk SSSR" Vol LXXXIV, No 5, pp 993-996

Butlerov's theory of the chem structure of org mols
does not imply strict linear additivity of bond
energies. Using a new math treatment, thermo-
dynamic eqs for the detn of vibrational energy,
rotational energy, and for the sum of the 2 are de-
rived for any hydrocarbon $C_nH_{2n} + 2$. The energies
of vibration and rotation of $C-C$ and $C-H$ bonds are
tabulated. Presented by Acad A. N. Frumkin 18 Apr
52.   223T19

MASLOV, P. G.

Oct 52

USSR/Chemistry - Propellants

"The Relationship Between the Specific Heat C_p^o of Alkylcycloalkanes, Temperature, and Length of the Hydrocarbon Chain," P.G. Maslov

DAN SSSR, Vol 86, No 4, pp 767-770

The specific heats of a number of alkylcycloalkanes were calcd using a formula that was derived. The length of the chain and the number of carbon atoms are taken into account. Presented by A. N. Frumkin 29 Jul 52.
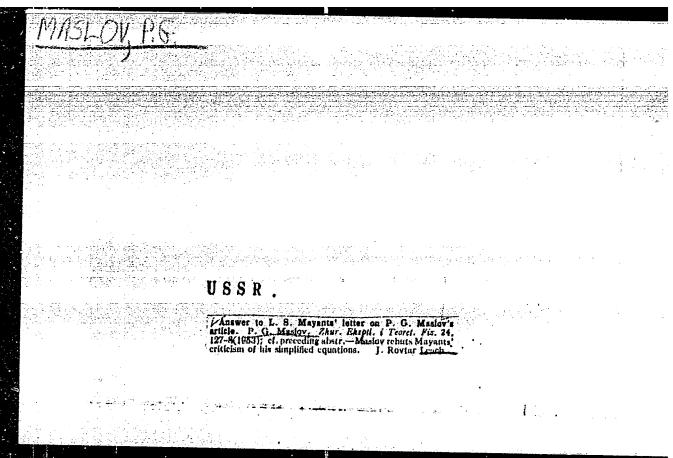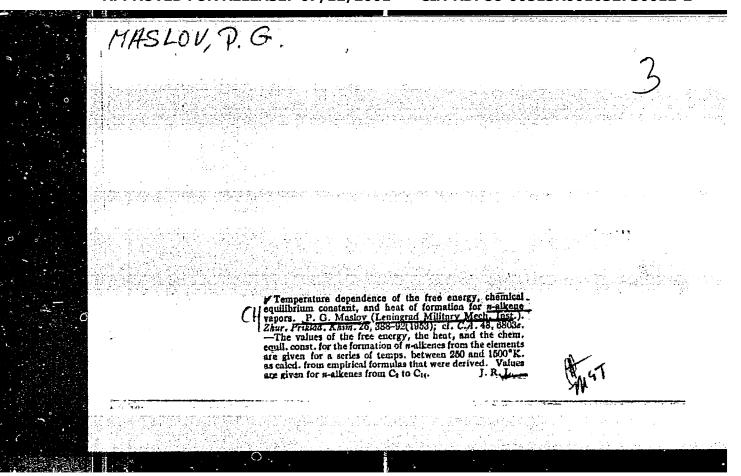
Source 264T20

MASLOV, P.G.

General formula for the free energy of formation of normal-alkane vapors from the elements. Doklady Akad. Nauk S.S.S.R. 86, 981-4 '52.
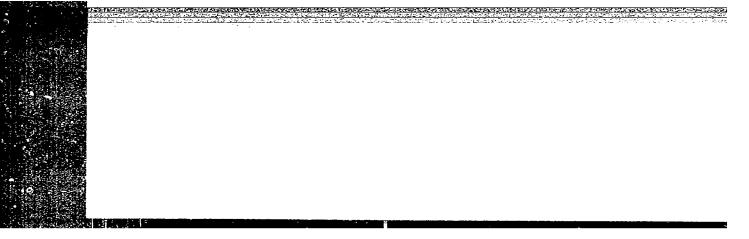(CA 47 no.13:6242 '53)

(MLRA 5:11)

MASLOV, P. G.

Physical Chemistry

Dissertation: "Vibrations of Molecules and the Thermodynamic Properties of Vapors of Organic Compounds." Dr Phys-Math Sci, Moscow State Pedagogical Inst imeni V. I. Lenin, Moscow, 1953. (Referativnyy Zhurnal—Khimiya, Moscow, No 3, Feb 54)

SO: SUM 213, 20 Sept 1954

MASLOV, P.G.

U S S R .

Answer to L. S. Mayants' letter on P. G. Maslov's article. P. G. Maslov, Zhur. Eksptl. i Teoret. Fiz. 24, 127-8(1953); cf. preceding abstr.—Maslov rebuts Mayants' criticism of his simplified equations.   J. Rovtar Leach

MASLOV, P. G.

3

Temperature dependence of the free energy, chemical equilibrium constant, and heat of formation for n-alkene vapors. P. G. Maslov (Leningrad Military Mech. Inst.). Zhur. Priklad. Khim. 26, 388-92(1953); cf. C.A. 48, 8803e. —The values of the free energy, the heat, and the chem. equil. const. for the formation of n-alkenes from the elements are given for a series of temps. between 250 and 1500°K. as calcd. from empirical formulas that were derived. Values are given for n-alkenes from C_2 to C_{16}.   J. R. L——

MASLOV, P. G.

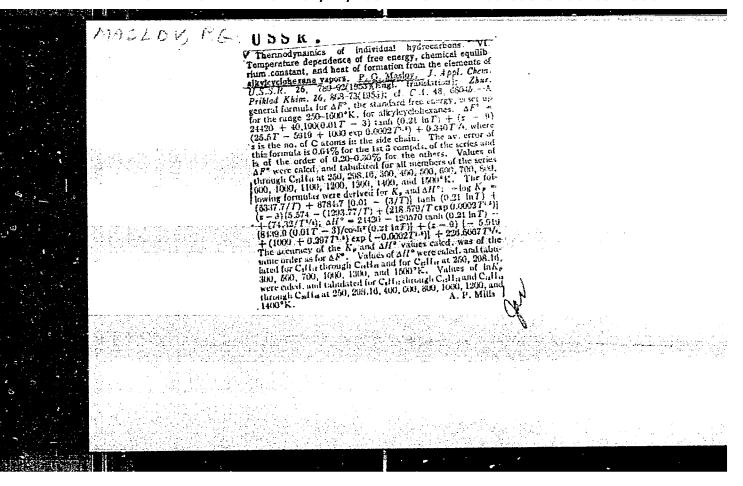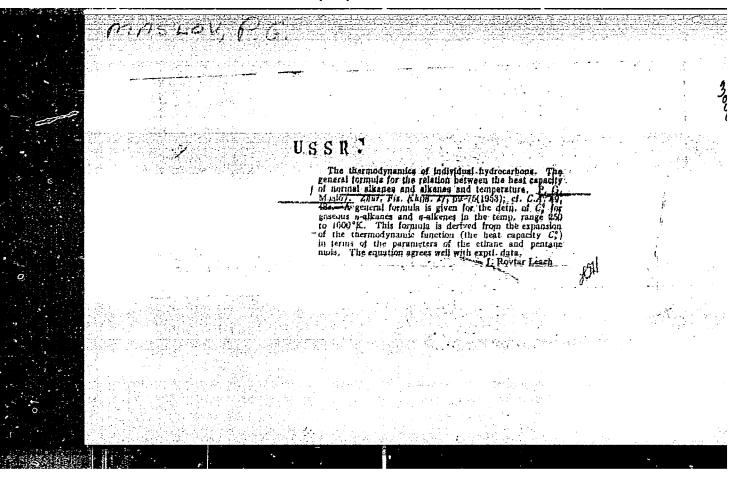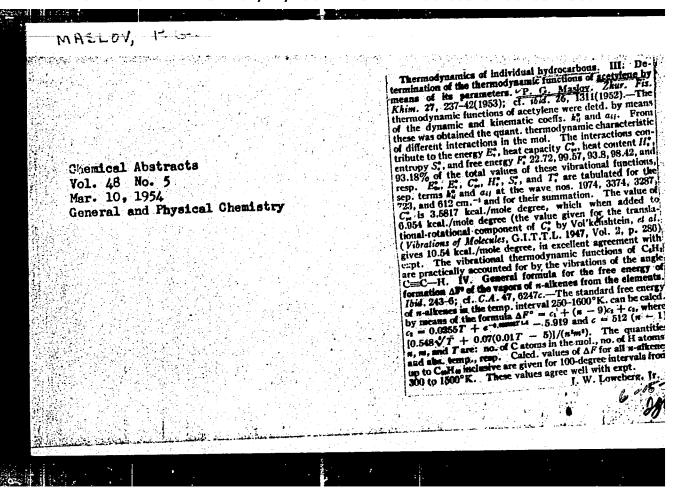Thermodynamics of individual hydrocarbons. IV. The temperature dependence of free energy, equilibrium constant, and heat of formation on the elements for N-alkylbenzenes. P. G. Maslov (Leningrad Military Mech. Inst.). Zhur. Priklad. Khim. 26, 543-6(1953).—A general formula for ΔZ°, the standard free energy, is set up for the range 250–1600°K. for n-alkylbenzenes. $\Delta Z^\circ = 45310 + 30094(0.01 T - 3)\tanh(0.2 \ln T) + (n - 9)[25.5 T - 5919 + 1000 e^{-x.xxxT}] + 9958(n - 5)[(n - 4)^x (m - 4)^x]\sqrt{T}$, where n and m are the no. of atoms of C and H in the mol., resp. and x is the no. of C atoms in the side chain. This formula gives ΔZ° for benzene, toluene, and ethylbenzene to errors of 0.50%, 0.54%, and 0.75%, resp., and for the others to 0.1%–0.2%. From the relation $\log K_p = -\Delta Z^\circ/4.575 T$ is derived the expression $-\log K_p = 9903.8 T^{-1} + 6577.9[0.01 - 3 T^{-1}\tanh 0.2 \ln T] + (x - 9)(5.574 - 1293.98 T^{-1} + 218.614 T^{-1} e^{-x.xxxT}) + 2148.1(n - 5)[(n - 4)^x (m - 4)^x] T^{-1/2}$. The accuracy is of the same order as for ΔZ°. The expression for ΔH° is $\Delta H^\circ = 45,300 - 90,282\tanh(0.2 \ln T) - 6018.8(0.01 T - 3)\cosh^2(0.2 \ln T) + (x - 9)[-5919 + (1000 + 0.297 T^2) e^{-x.xxxT}] + 7466.67(n - 5)[(n - 4)^x (m - 4)^x]\sqrt{T}$. This formula is similar to one found in the case of n-alkenes (Zhur. Priklad. Khim. 26, 4, 388-02(1953)). Only the numerical coeffs. are different. This suggests that CH_2 groups make contributions in similar ways in all org. compds. The data for ΔH° at 293.16° are as good as any in the literature. Data for other temps. are not reported in the literature. Joseph B. Levy

MASLOV, P.G.

Thermodynamics of individual hydrocarbons. V. A single law of the temperature dependence of free energy and the constant of chemical equilibrium of vapors of alkyl-cyclopentanes. P. G. Maslov. Zhur. Priklad. Khim. 26, 749-62 (1953); cf. C.A. 48, 4844d; preceding abstrs.— Math. study of the temp. dependence of the free energy and the equil. const. of alkylcyclopentane vapors in the temp. interval of 250-1600°K. The av. errors of detns. for cyclopentane, methylcyclopentane, and ethylcyclopentane were 0.69, 0.64, and 0.82% resp., and for the remaining alkylcyclopentanes was of the order of 0.10-0.40%. The data obtained agreed well with the latest most reliable spectroscopic calcns. in the literature. Gladys S. Macy

MASLOV, P.G.

USSR.

V Thermodynamics of individual hydrocarbons. VI.
Temperature dependence of free energy, chemical equilibrium constant, and heat of formation from the elements of alkylcyclohexane vapors. P. G. Maslov. J. Appl. Chem. U.S.S.R. 26, 783-92(1953)(Engl. translation); cf. C.A. 48, 6804b.--A general formula for ΔF°, the standard free energy, is set up for the range 250–1600°K. for alkylcyclohexanes. $\Delta F^\circ = 24420 + 40.190(0.01T - 3) \tanh (0.21 \ln T) + (z - 9)(25.5T - 5910 + 1000 \exp 0.0002T^{1.4}) + 0.340T^2$, where z is the no. of C atoms in the side chain. The av. error of this formula is 0.64% for the 1st 6 compds. of the series and is of the order of 0.20-0.30% for the others. Values of ΔF° were calcd. and tabulated for all members of the series through C_9H_{18} at 250, 298.16, 300, 400, 500, 600, 700, 800, 900, 1000, 1100, 1200, 1300, 1400, and 1500°K. The following formulas were derived for K_p and ΔH°: $-\log K_p = (6337.7/T) + 8784.7 [0.01 - (3/T)] \tanh (0.21 \ln T) + (z - 9)[5.574 - (1293.77/T) + (218.579/T \exp 0.0002T^{1.4})] - (74.32/T^{1/2})$; $\Delta H^\circ = 24420 - 120570 \tanh (0.21 \ln T) + (8149.0 (0.01T - 3)/\cosh^2(0.21 \ln T)] + (z - 9) [- 5910 + (1000 + 0.397T^{1.4}) \exp (-0.0002T^{1.4})] + 226.6607T^2/.$ The accuracy of the K_p and ΔH° values calcd. was of the same order as for ΔF°. Values of ΔH° were calcd. and tabulated for C_7H_{14} through C_9H_{18} and for C_6H_{12} at 250, 298.16, 300, 400, 700, 1000, 1300, and 1500°K. Values of $\ln K_p$ were calcd. and tabulated for C_7H_{14} through C_9H_{18} and C_6H_{12} through C_9H_{18} at 250, 298.16, 400, 600, 800, 1000, 1200, and 1400°K.
A. P. Mills

MASLOV, P. G.

USSR/Chemistry - Thermodynamics, Aug 53
Hydrocarbons

Temperature Dependence of Free Energy, Equili-
brium Constants, and Heats of Formation From
the Elements of n-Alkylcyclohexane Vapors,"
P.G. Maslov

Zhur Prik Khim, Vol 26, No 8, pp 868-873

Proposes single formulas for temp dependence of
free energy, equil consts, and heats of formation
for n-alkylcyclohexanes in the vapor phase over
the temp range 250-1600°K. The results were found
to be in good agreement with the latest calcs
based on spectroscopic data.

273T32

MASLOV, P. G.

USSR

The thermodynamics of individual hydrocarbons. The general formula for the relation between the heat capacity of normal alkanes and alkenes and temperature. P. G. Maslov. Zhur. Fiz. Khim. 27, 75-76(1953); cf. C.A. 49, 48e.—A general formula is given for the detn. of C_p for gaseous n-alkanes and n-alkenes in the temp. range 250 to 1600°K. This formula is derived from the expansion of the thermodynamic function (the heat capacity C_p°) in terms of the parameters of the ethane and pentane mols. The equation agrees well with exptl. data.
L. Rovtar Leach

1. MASLCV, P. G.

2. USSR (600)

4. Thermodynamics

7. Dependence of free energy, chemical equilibrium constants and heat:
    of formation of vapors of n-alkynes on temperature, Zhur. prikl.
    khim., 27, No. 2, 1953.

9. Monthly List of Russian Accessions, Library of Congress, ___April,___ 1953, Uncl

MASLOV, P. G.

Thermodynamics of individual hydrocarbons. III. Determination of the thermodynamic functions of acetylene by means of its parameters. P. G. Maslov. Zhur. Fiz. Khim. 27, 237-42(1953); cf. ibid. 26, 1311(1952).—The thermodynamic functions of acetylene were detd. by means of the dynamic and kinematic coeffs. k_{ii}^o and a_{ii}. From these was obtained the quant. thermodynamic characteristic of different interactions in the mol. The interactions contribute to the energy E_i^o, heat capacity C_{vi}^o, heat content H_i^o, entropy S_i^o, and free energy F_i^o 22.72, 99.57, 93.8, 98.42, and 93.18% of the total values of these vibrational functions, resp. E_v^o, E_i^o, C_{vi}^o, H_i^o, S_i^o, and T_i^o are tabulated for the sep. terms k_{ii}^o and a_{ii} at the wave nos. 1074, 3374, 3287, 723, and 612 cm.$^{-1}$ and for their summation. The value of C_v^o is 3.5817 kcal./mole degree, which when added to 0.954 kcal./mole degree (the value given for the translational-rotational component of C_v^o by Vol'kenshtein, et al., (Vibrations of Molecules, G.I.T.T.L. 1947, Vol. 2, p. 280) gives 10.54 kcal./mole degree, in excellent agreement with expt. The vibrational thermodynamic functions of C_2H_2 are practically accounted for by the vibrations of the angle $C\equiv C-H$. IV. General formula for the free energy of formation ΔF^o of the vapors of n-alkenes from the elements. Ibid. 243-6; cf. C.A. 47, 6247c.—The standard free energy of n-alkenes in the temp. interval 250-1600°K. can be calcd. by means of the formula $\Delta F^o = c_1 + (n - 9)c_2 + c_3$, where $c_1 = 0.0255T + e^{-1.035T}$ = −5.919 and $c = 512 (n - 1)$ [0.548$\sqrt{T}$ + 0.07(0.01T − 5)]/($n^{1/2}m^2$). The quantities n, m, and T are: no. of C atoms in the mol., no. of H atoms and abs. temp., resp. Calcd. values of ΔF for all n-alkenes up to C_9H_{18} inclusive are given for 100-degree intervals from 300 to 1600°K. These values agree well with expt.
J. W. Loweberg, Jr.

1. MASLOV, P. G.

2. USSR (600)

4. Olefins

7. Thermodynamics of individual hydrocarbons. Part 4. General formula for the
   free energy ΔZ^o of the formation of n-alkenes from elements. Zhur. fiz. khim.
   27, No. 2, 1953.

9. Monthly List of Russian Accessions, Library of Congress, _____April_____ 1953, Uncl

MASLOV, P.G.

The Committee on Stalin Prizes (of the Council of Ministers USSR) in the fields of science and inventions announces that the following scientific works, popular scientific books, and textbooks have been submitted for competition for Stalin Prizes for the years 1952 and 1953. (Sovetskaya Kultura, Moscow, No. 22-40, 20 Feb - 3 Apr 1954)

Name	Title of Work	Nominated by
Maslov, P.G.	"Certain Problems of the Theory of Vibration of Molecules and a Generalization of the Thermodynamic Properties of Organic Compounds"	Leningrad Military Mechanical Institute

SO: W-30604, 7 July 1954

MASLOV, P.G.

USSR/Chemistry - Physical chemistry

Card 1/1   Pub. 147 - 20/27

Authors   : Maslov, P.G.; Prevratukhin, V.D.; Danilov, Yu. V.; and Lychagin, A.A.

Title   : Oscillatory spectra of n-pentane

Periodical : Zhur. fiz. khim. 28/2, 328-336, Feb 1954

Abstract   : The symmetry of an n-pentane C_5H_{12} molecule and the coefficients of its effect were determined. The basic frequencies of n-pentane were calculated and the interpretations are given in tables. It was confirmed (through calculation), that the number of valent oscillation frequencies of $C - H^1$ bonds should be at least seven and not four as mentioned in literature. It was found that the oscillation frequencies of C - C bonds of the linear C - C - C - C - C chain were, to a greater extent, generated by the oscillations of the C - C - C (φ) components and their reaction with the C - C bonds. Thirteen references: 9-USSR; 3-USA and 1-German (1935-1952). Tables; diagram.

Institution : ....
Submitted   : May 8, 1953

MASLOV, P.G.

U S S R .

Thermodynamics of individual hydrocarbons. V. A
single law of the temperature dependence of free energy
and the constant of chemical equilibrium of vapors of alkyl-
cyclopentanes. P. G. Maslov. *J. Appl. Chem. U.S.S.R.*
26, 609-811 (1954)(Engl. translation).—See *C.A.* **48**, 6804b.
H. L. H.

MASLOV, P. G.

USSR/Chemistry

Card 1/1

Author   : Maslov, P. G.

Title   : The role of reactions during molecular oscillations

Periodical : Zhur. Fiz. Khim., 28, Ed. 5, 873 - 882, May 1954

Abstract   : The role of reactions during molecular oscillations was investigated. An
               approximate estimation was made of the role of mutual effects of structural
               groups on the thermodynamic properties of a substance during molecular os-
               cillations. It was determined that reactions play a highly important and
               even decisive role in thermodynamic property values of substances. Four
               USSR references. Tables, graphs.

Institution : ...

Submitted   : Sept. 23, 1953

Role of interaction in the ethane-d_6 molecule. P. G. Maslov. Zhur. Fiz. Khim. 28, 1507-20(1954); cf. C.A. 49, 60776.—Increments of the vibrational (v.) null energy, v. enthalpy (H), v. heat capacity (C), v. free energy (F), and v. entropy (S) of the C_2D_6 (I) mol. due to each of its parameters at 293.16°K. are tabulated for wave nos. between 600 and 2300 cm.$^{-1}$, as are the total values for each of kinematic and dynamic interaction in the I mol. V. interactions contribute 35, 82, 84, 84, and 84% of the total functions v. energy, C, H, S, and F, resp. The energies of the C—C and C—D bonds in I consist largely of interaction energy. — J. W. Loweberg, Jr.

MASLOV, P.G.

Single formulas for the determination of molecular refraction,
dispersion, parachors, and viscosity of organic compounds at
given external conditions. Dokl.AN SSSR 94 no.6:1105-1108 F
'54.   (MLRA 7:2)

1. Leningradskiy voyenno-mekhanicheskiy institut.
                              (Chemistry, Physical and theoretical)

MASLOV, T.G

AID P - 2291

Subject   : USSR/Chemistry

Card 1/1 Pub. 152 - 17/21

Author   : Maslov, P. G.

Title   : Single formulas for determination of Kerr constants of
n-alkanes and n-alkenes

Periodical: Zhur. prikl. khim., 28, no.3, 328-330, 1955

Abstract : Calculations were carried out for determination of the
constants of n-alkanes (in vapor and liquid phase).
Experimental data obtained by the author are compared
with data from literature. Three tables, 6 references
(all Russian: 1941-1952).

Institution: Leningrad Military Mechanical Institute

Submitted : Ap 9, 1953

MASLOV, P. G

Subject   : USSR/Chemistry

Card 1/1   Pub. 152 - 18/21

Author   : Maslov, P. G.

Title   : Graphic method for calculating the heat capacities of
              organic compounds

Periodical: Zhur. prikl. khim., 28, no.3, 330-333, 1955

Abstract   : A simple and exact method for the determination of heat
              capacities of vapors of organic compounds is described.
              One diagram, 9 references (all Russian: 1945-1953).

Institution: Leningrad Military Mechanical Institute

Submitted : N 20, 1953

MASLOV, P. G.

USSR/ Chemistry - Physical chemistry

Card 1/2   Pub. 147 - 8/26

Authors   :   Maslov, P. G.

Title   :   Graphical methods of determining the thermodynamic characteristics
                  of organic compounds

Periodical   :   Zhur. fiz. khim. 29/1, 62-69, Jan 1955

Abstract   :   The introduction of a very simple but highly accurate graphical
                  method for the determination of chemical equilibrium constants of the
                  formation of organic compounds of normal structure in a temperature
                  range of from 250 - 3000 K is announced. Also introduced were: a
                  simple but quite accurate graphical method for the determination of
                  isobaric-isothermal potentials of the formation of vapors of organic
                  compounds in the very same temperature range and for establishing
                  the heats of formation of vapors of organic compounds of normal
                  structure.

Institution: .....

Submitted   :   April 1, 1954

Periodical : Zhur. fiz. khim. 29/1, 62-69, Jan 1955

Card 2/2   Pub. 147 - 8/26

Abstract : The methods were found to be effective for the solid and liquid states of a given substance as well as for vapors of oxygen-and nitrogen containing org. substances and for mecaptan compounds. Twelve USSR references (1949-1954. Graphs.

MASLOV, P.G.

Regularities in thermodynamic properties of liquid-phase organic compounds.
Zhur.fiz.khim. 29 no.4:718-722 Ap '55.   (MIRA 8:8)
      (Thermochemistry) (Chemistry, Organic)

Maslov, P G

AUTHORS: Maslov, P. G.   and   Maslov, Yu. P.

TITLE: On the Possibility of Prediction of Vibrational Spectra
             of some Compounds from the Known Spectra of Other Compounds.
             (O vozmozhnosti predskazaniya kolebatel'nykh spektrov
             odnikh soyedineniy po izvestnym spektram drugikh).

ABSTRACT: Formulae of halogen derivatives of methane can be obtained
             as combinations of chemical formulae of other methane
             derivatives, e.g. $CHXY_2 = 0.5(CHY_3 + CHYX_2)$, where
             X, Y, are halogens. Knowing vibrational spectra (v.s.)
             for molecules CHY_3 and $CHXY_2$ and averaging their
             frequencies, one can obtain a good approximation to the
             v.s. of $CHYX_2$. Table 1 gives frequencies of v.s. of
             halogen derivatives of methane calculated in this way.
             These calculated values are compared with experimental
             ones and are found to be in good agreement.   Tables 2,
             4, 5, 6, 7, 9 and 10 give values of vibration frequencies
Card 1/3   calculated in this way for methane halides, ethane halogen

51-1-6/18

On the Possibility of Prediction of Vibrational Spectra of some
Compounds from the Known Spectra of Other Compounds.

derivatives, trimethylene halides, halogenated ethylenes,
ethylene halides, certain simple molecules like SeF_6,
$GeCl_4$ and other compounds.   Tables 3, 8 and 12 give
vibrational thermodynamic functions calculated from
vibration frequencies both obtained experimentally and
determined in the way indicated above.   From the
results obtained the authors conclude that v.s. frequencies
of the molecules discussed are approximately additive.
This also applies to their intensities and polarizations.
The spectra calculated by averaging are thermodynamically
almost equivalent to the true spectra.   In the majority
of cases the spectra calculated by averaging have
frequencies which are nearly identical with those
calculated using the theory of molecular vibrations,
and are close to the experimental values.   The method
proposed in this paper can be applied to frequency
harmonics as well.   There are 12 tables, and 18

Card 2/3   references, 3 of which are Slavic.

51-1-6/18

·On the Possibility of Prediction of Vibrational Spectra of some
Compounds from the Known Spectra of Other Compounds.
ASSOCIATION: Leningrad Military Mechanical Institute, Department of
           Physics. (Leningrad voyenno-mekhanicheskiy institut,
           Kafedra fiziki.)

SUBMITTED: December 25, 1956.

AVAILABLE:

Card 3/3

MASLOV, P. G.

USSR/Atomic and Molecular Physics - Statistical Physics   D-3
Thermodynamics.

Abs Jour   : Ref Zhur - Fizika, No 1, 1958, 737

Author   : Maslov, P.G.
Inst   : —
Title   : Concerning Methods of Determining the Specific Heats of
Vapors of Organic Compounds.

Orig Pub   : Zh. prikl. khimii, 1957, 30, No 5, 736-744

Abstract   : On the basis of theory of vibration of molecules, the au-
thor derives unified refined formulas for the determina-
tion of the standard molar specific heats C_p^o for vapors
of n-alkanes, n-alkenes, n-alkines, n-alkylbenzols, n-al-
kylcyclohexanes, n-alcohols, aldehydes, acids, ethers,
mercaptanes, and thio-ethers over a wide range of tempe-
ratures. The formulas show explicitly the term respon-
sible for the fraction of the specific heat die to the
methylene group CH_λ. The results are compared with the

Card 1/2

USSR/Physical Chemistry - Kinetics, Combustion, Explosions, Topo-
            chemistry, Catalysis.   B-9

Abs Jour: Referat. Zhurnal Khimiya, No 3, 1958, 7222.

Author : P.G. Maslov.
Inst   :
Title   : Graphic Method of Determination of Combustion Temperatures
          of Organic Compounds.

Orig Pub: Zh. fiz. khimii, 1957, 31, No 5, 1063-1071.

Abstract: A graphic calculation method of combustion temperatures of or-
          ganic compounds in open vessels is described. This method is
          based on the assumption of additivity by methylene groups of
          all terms of the heat balance equation, and uses thermal data
          for two members of the homologous series in question. Examples
          of practical application of the method are given. See also
          RZhKhim, 1956, 53870; 1957, 50652, 65642.

Card   : 1/1   -21-

AUTHOR: Maslov, P. G.   SOV/78-3-12-5/36

TITLE: The Determination of the Thermo-Chemical Radii of Ions (K
               opredeleniyu termokhimicheskikh radiusov ionov)

PERIODICAL: Zhurnal neorganicheskoy khimii, 1958, Vol 3, Nr 12,
               pp 2618-2620 (USSR)

ABSTRACT: A new method for determining the thermo-chemical radii of ions
               is described which gives as high a degree of accuracy as those
               methods previously known. The formula $r_x = (a+bn)Å$ is used in
               carrying out the calculations. The thermo-chemical radii r_x
               (in Å) for cations of the type $[Ca(H_2O)n]^{2+}$, $[Mg(H_2O)n]^{2+}$,
               $[Sr(H_2O)n]^{2+}$, $[Ba(H_2O)n]^{2+}$ and $[Li(H_2O)n]^{2+}$ were calculated with
               great accuracy using equation (1). The thermo-chemical radii
               of the complex ions $[Ba(NH_3)m]^{2+}$, $[Sr(NH_3)m]^{2+}$, $[Au(NH_3)m]^{2+}$,
               $[Cd(NH_3)m]^{2+}$, $[Co(NH_3)m]^{2+}$ and $[Cu(NH_3)m]^{2+}$ were also calculated.
               The thermo-chemical radii of various halogen derivative ions

Card 1/3   of the type $BH_i F_j Cl_k Br_q J_r \cdot mQ$ were easily and exactly calculated

The Determination of the Thermo-Chemical Radii of Ions

using the following equation:

$$A_{BH_iF_jCl_kBr_qJ_r^{\delta\pm}} = \frac{1}{n}(iA_{BH_n^{\delta\pm}} + jA_{BF_n^{\delta\pm}} + kA_{BCl_n^{\delta\pm}} + qA_{BBr_n^{\delta\pm}} + $$

$$+ rA_{BJ_n^{\delta\pm}})\quad (13a).$$

The ionic radius of $\left[HgF_iCl_jBr_kJ_q\right]^{2-}$, for example, was one of those calculated. From the thermo-chemical radii of the complex ions JO_3^-, ClO_3^-, PO_4^{3-} and SbO_4^{3-} the radii r_x of the BrO_3^- and AsO_4^{3-} ions can be calculated using equations (14) and (15):

$$r_{BrO_3^-} = 0.5(r_{JO_3^-} + r_{ClO_3^-})\qquad (14)$$

$$r_{AsO_4^{3-}} = 0.5(r_{PO_4^{3-}} + r_{SbO_4^{3-}}).\qquad (15)$$

The calculation of the thermo-chemical radii for other groups of ions was also carried out. There are 1 table and 9 references, 7 of which are Soviet.

Card 2/3

SOV/78-3-12-5/36

The Determination of the Thermo-Chemical Radii of Ions

SUBMITTED: November 22, 1957

Card 3/3

AUTHORS: Maslov, P. G. and Maslov, Yu. P.

TITLE: Heat of Formation of Halogen-Substituted Methane and
                Ethylene (Teploty obrazovaniya galoidzameshchennykh
                metana i etilena)

PERIODICAL: Khimiya i Tekhnologiya Topliv i Masel, 1958, Nr 10,
                pp 50 - 55 (USSR)

ABSTRACT: The authors recently described a method for calculating
                the thermodynamic properties of halogen-substituted
                methane and other compounds (Ref.10) at temperatures
                varying between 100 to 1500°K, and now give details of
                a method for calculating the heat of formation ΔH^0_f
                for halogen-substituted methane and ethylene at
                25°C. Results obtained by this method conform with
                data given by other authors (Refs.13 - 25). The accu-
                racy of the calculated results varies between 0 to 5%,
                and in some cases 10%. The heats of formation of halo-
                substituted methane in the gaseous phase at 25°C (in
                ccal/mole) (Table 1) and for halo-substituted ethylenes
                in the gaseous phase at 298.16°K (Table 2) are given.
                The authors suggest that their calculation is sufficient-
                ly accurate for experimental purposes. They also ascer-
Card 1/2   tain the heats of formation of bromine, iodine and

SOV/65-58-10-11/15

Heat of Formation of Halogen-Substituted Methane and Ethylene

fluorine-substituted ethylene which have not previously
been described in literature (Table 2). There are 2
Tables and 25 References: 13 English, 10 Soviet and
2 German.

Card 2/2

AUTHORS: Maslov, P. G., Klochikhin, A. A.   79-28-3-58/61

TITLE: Molecular Refractions of Some Classes of Alkylthiophenes and
                Alkylthiacycloalkanes (Molekulyarnyye refraktsii nekotorykh
                klassov alkiltiofenov i alkiltiatsikloalkanov)

PERIODICAL: Zhurnal Obshchey Khimii, 1958, Vol. 28, Nr3, pp. 835-838
                (USSR)

ABSTRACT: In connection with earlier works the present work proposes
                uniform formulae hitherto unknown for the determination of
                the molecular refractions (R) of alkylthiophenes, alkylthia-
                cyclopropanes, alkylthiacyclopentanes and alkylthiacyclo-
                hexanes. As is known in homologous series of organic compounds
                ending with a cycle (cyclopentanone etc.) the additivity of
                many properties in the methylene groups CH_2, starting already
                from the second representative of this series, is practically
                well accomplished. This can without difficulty also be found
                with molecular refraction. The computation of the molecular
                refractions of the two low alkylthiophenes according to the
                molecular refraction of the 2-propylthiophene (equal to 38,64
                at $20°$ C) is mentioned as example (reference 1). With con-

Card 1/2

Molecular Refractions of Some Classes of Alkylthiophenes and   79-28.3-58/61
Alkylthiacycloalkanes

sequent subtraction of that part of the molecular refraction
pertaining to a CH_2 group the following figures are obtained:
for the 2-ethylthiophene 34,005, for the 2-methylthiophenone
29,37, for thiophene 24,735. The obtained values differ from
the experimental data of the molecular refractions of these
compounds by 0,095, 0,08 and 0,37, or by 0,3, 0,25 and 1,5%
respectively. From the conclusions drawn from this it is poss-
ible to set up general rules for the determination of R of
every other representative of the respective compound series
according to the values for the molecular refraction given in
reference 1 for the third and in particular for the fourth
member of the homologous series of the sulfurorganic com-
pounds. The mentioned molecular refractions of some 2-alkyl-
and 3-alkylthiophenes as well as the two tables serve as
general survey. There are 2 tables and 8 references, 7 of
which are Soviet.

ASSOCIATION: Leningradskiy voyenno-mekhanicheskiy institut
                 (Leningrad Military Mechanical Institute)

SUBMITTED: July 10, 1956

Card 2/2

AUTHORS: Maslov, Yu. P., Maslov, P. G.   SOV/76-32-8-4/37

TITLE: A Method of Calculating the Thermodynamic Properties of Some
                Compounds Without Knowing Their Vibration Spectra (Metod
                rascheta termodinamicheskikh svoystv nekotorykh soyedineniy
                bez znaniya ikh kolebatel'nykh spektrov)

PERIODICAL: Zhurnal fizicheskoy khimii, 1958, Vol. 32, Nr 8,
                pp. 1715-1725 (USSR)

ABSTRACT: The possibility of applying this method to organic and inorganic
                compounds is investigated. It is based on the knowledge of the
                structure and the vibration spectra of the molecules of other,
                sometimes more simple compounds, which generally seen may also
                belong to another homologous series. The halogen derivatives
                of methane, ethane, ethylene, ethine, and other compounds offer
                good prospects for this method. Also compounds in which one or
                several atoms were substituted by atoms of the elements belong-
                ing to one of the side chains of the D. I. Mendeleyev table
                belong to these compounds. The problem is to find the values
                of a thermodynamic property A for the entire family of com-
                pounds, with the quantity A being known only for some simple
Card 1/2   representatives of this family (on the same conditions). Some

SOV/76-32-8-4/37

A Method of Calculating the Thermodynamic Properties of Some Compounds
Without Knowing Their Vibration Spectra

data of each single representative of the whole family must
be known, however, or it must be possible to calculate   them.
In the calculations carried out the data by Pitzer (Pitser)
(Refs 1, 7), Pitzer and Gwinn (Gvin) (Ref 7), as well as by
Pitzer and Gelles (Ref 8) are mentioned. This way the thermo-
dynamic properties as well as the heat capacity and the entropy
of a number of the halogen hydrocarbons mentioned above were
calculated. The results obtained agree with those mentioned in
reference 8; they are given in a table. There are 6 tables
and 17 references, 8 of which are Soviet.

SUBMITTED: November 29, 1956

Card 2/2

AUTHOR: Maslov, P. G.   SOV/76-32-9-17/46

TITLE: A Contribution to Methods for Calculating the Equilibrium
             Composition of Combustion Products of Mixtures With Excess
             Oxygen (K metodam rascheta ravnovesnogo sostava produktov
             sgoraniya smesey pri izbytke kisloroda)

PERIODICAL: Zhurnal fizicheskoy khimii, 1958, Vol 32, Nr 9,
             pp 2061 - 2067 (USSR)

ABSTRACT: The author suggests a new method of calculation which is
             simpler than those already known (Refs 1 to 16). This
             method is valid to at least $3500°$ K and for $\alpha > 1,05$.
             The author has in this paper worked out the method for
             the elements carbon, nitrogen, hydrogen, and oxygen, but
             the method is suitable also for a great number of
             elements; in the case of these other elements naturally
             the formulae more complicated. In place of oxygen another
             oxidant can also be used. A table compares the calculation
             according to the method of the author with the calculation
             by A.M.Gurvich and Yu.Kh.Shaulov (Ref 10). There are
             1 table and 17 references, 13 of which are Soviet.

Card 1/2

A Contribution to Methods for Calculating the   SOV/76-32-9-17/46
Equilibrium Composition of Combustion Products of Mixtures With Excess
Oxygen

ASSOCIATION: Voyenno-mekhanicheskiy institut, Leningrad (Leningrad
               Military-Mechanical Institute)

SUBMITTED: November 28, 1956

Card 2/2

MASLOV, P. G.

"On the Application of the Additive-Statistic Method to the Study of
Absorption and Fluorescence Spectra."

report submitted but not presented at the 4th International Meeting of Molecular
Spectroscopy, Bologna, Italy, 7-12 Sept 1959.

Leningrad University, USSR.

5(2), 5(4), 24(8)   SOV/153-2-3-5/29

AUTHOR: Maslov, P. G.

TITLE: IX. Thermodynamical Properties of Chemical Compounds
               Containing Mercury

ABSTRACT: The corresponding values of the mixed halides (HgFCl etc)
               were computed according to the method described in reference 5,
               developed by Yu. Maslov from the values given in publications
               for the heat of formation, free energy, entropy, and specific
               heat of the mercury (I)-, of the mercury (II) halides, and of
               the tri- and tetra halide complex ions (Table 1). Furthermore,
               the heats of a formation of numerous complex compounds were
               computed (Tables 2, 3, and 4) from the values for the more
               simple complex compounds. As far as data from publications were
               available they are in good agreement with the values computed,
               the error being in the order of magnitude between 0.5 and 5 %.
               Approximation formulas for the computation of the heats of
               formation were set up for the crystal hydrates and ammoniacates
               (Table 5). Besides, also approximation formulas were found

Card 1/2

IX. Thermodynamical Properties of Chemical Compounds   SOV/153-2-3-5/29
Containing Mercury

        permitting the computation of the free energy, the
        logarithm of the equilibrium constant, the entropy, and the
        specific heat (Formulas 2-5) for the crystal hydrates. There
        are 5 tables and 8 references, 5 of which are Soviet.

ASSOCIATION: Leningradskiy voyenno-mekhanicheskiy institut-Kafedra fiziki
        (Leningrad Military-mechanical Institute, Chair of Physics)

SUBMITTED: September 12, 1957

Card 2/2

SOV/51-7-3-11/21

AUTHOR: Maslov, P.G.

TITLE: On the Use of the Additive-Statistical Method in the Studies of
           Absorption and Fluorescence Spectra.

PERIODICAL: Optika i spektroskopiya, 1959, Vol 7, Nr 3, pp 355-365 (USSR)

ABSTRACT: Ultraviolet absorption and fluorescence spectra are of considerable
           interest but their experimental determination is frequently difficult
           and sometimes impossible (Ref 1). Consequently theoretical methods of
           calculation of fluorescence and absorption spectra would be very useful.
           The present paper shows that it is possible to use Yu.P. Maslov and the
           present author's additive-statistical method (Refs 3-5) to obtain
           electron absorption and fluorescence spectra of organic compounds. The
           frequencies of the fundamental, combination and torsional vibrations, as
           well as other physico-chemical properties of families of similar compounds,
           can be calculated from the properties of the simpler members of the family
           using

$$B_i = \frac{1}{s_0} \sum_j \delta_j B_j \qquad (1)$$

Card 1/2   where B is the value of frequency or other property of the substance,

On the Use of the Additive-Statistical Method in the Studies of Absorption and Fluorescence Spectra

$s_0 = \sum_j b_j$ is the valence of a group common to all members of the family studied and b_j is a numerical coefficient of B_j. This basic formula was employed to obtain relationships for calculation of various properties of the electron spectra, such as position, intensity, quantum yield, etc., assuming that the effects of various substituents are additive. The relationships are shown to be in satisfactory agreement with experiment for a large group of aromatic compounds: Table 1 gives the calculated and experimental values of the ionization potentials of 28 organic compounds and the dipole moments of these organic compounds and HCl, HBr and HI, while Tables 2-5 give the calculated and experimental values of the absorption and fluorescence band maxima, the oscillator strengths and the quantum yields of solutions of anthracene derivatives. There are 5 tables and 30 references, 17 of which are Soviet, 9 English, 2 translations into Russian, 1 German and 1 Swiss.

SUBMITTED: December 22, 1958

Card 2/2

AUTHORS: Maslov, P. G., Maslov, Yu. P.   SOV/153-2-4-9/32

TITLE: Thermodynamic Properties of Compounds Containing Lanthanides

PERIODICAL: Izvestiya vysshikh uchebnykh zavedeniy. Khimiya i khimicheskaya
               tekhnologiya, 1959, Vol 2, Nr 4, pp 516 - 521 (USSR)

ABSTRACT: Although the compounds mentioned in the title are considered with
               great interest (Refs 1-3) their thermodynamic properties are
               but little investigated (Refs 1-3). Their investigation could
               be somewhat extended (Refs 4-10) by methods developed recently
               (Refs 4,5). In the paper under review the properties mentioned
               of the compounds containing lanthanides in crystalline state and
               in solutions at 25° are discussed. As is known, a given thermo-
               dynamic property A of any constituent of a group of related
               compounds, e.g. of halides of the type $BF_iCl_jBr_kJ_q$, can be computed
               with great accuracy according to formula (1); $n=i+j+k+q$; B = a
               group of atoms equal for all representatives of the group of
               compounds under discussion; BF_n, BCl_n, BBr_n and BJ_n are the
               simplest representatives of the group; the values of the thermo-
               dynamic property of the latter are known in advance and with
Card 1/3   sufficient accuracy. By using the method of reference 5, the

Thermodynamic Properties of Compounds Containing   SOV/153-2-4-9/32
Lanthanides

authors determined the formation heats $(-\Delta H^o{}_f)$, free energies
$(-\Delta Z^o{}_f)$, logarithms of the equilibrium constant $(\log K_f)$, and
entropies (S^o) of several halides of: scandium, yttrium, lute-
tium, thul, erbium, holmium, dysprosium, gadolinium, samarium,
neodymium, praseodymium, cerium, and lanthanum. The computation
results are shown in tables 1,2, and 4. Moreover, the authors
obtained approximate general formulas for the determination of
the formation heats, free energies, logarithms of the equilibrium
constant, entropy, and heat capacity $(C^o{}_p)$ of the groups of lan-
thanide crystallohydrates on account of the methods described in
references 5 and 11. These groups were: $X_2(SO_4)_3 \cdot nH_2O$ (X=Y, La,
Yb, Er, Ho, Dy, Tb, Gd, Eu, Sm, Nd, Pr, Ce, La). $XO_3 \cdot nH_2O$ (X= Nd,
Pr, Ce), $Er_2(C_2H_3O_2)_2 \cdot nH_2O$, and ammoniates $XCl_3 \cdot mNH_3$

(X= Sm, Nd, and Ce). All

these formulas are shown in table 5, Table 3 shows a comparison
of results computed by means of formulas with experimental data
Card 2/3   for several compounds. The results are in good agreement (accuracy

Thermodynamic Properties of Compounds Containing   SOV/153-2-4-9/32
Lanthanides

            of a magnitude of 0.2-1%). There are 5 tables, and 11 refer-
            ences, 10 of which are Soviet.

ASSOCIATION: Leningradskiy mekhanicheskiy institut, Kafedra fiziki (Lenin-
            grad Mechanics Institute, Chair of Physics)

SUBMITTED: September 1o, 1957

Card 3/3

5(4)

SOV/79-29-5-3/75

AUTHOR: Maslov, P. G.

TITLE: Thermodynamic   Properties   of Calcium-, Gallium-, Indium and Thallium Compounds (Termodinamicheskiye kharakteristiki kal'tsiyevykh, galliyevykh, indiyevykh i talliyevykh soyedineniy)

PERIODICAL: Zhurnal obshchey khimii, 1959, Vol 29, Nr 5, pp 1413 - 1423 (USSR)

ABSTRACT: In the present paper general approximate formulas were obtained according to the methods described in references 1-4 for the determination of formation heat $(-\Delta H_f^0)$, free energies $(-\Delta Z_f^0)$, logarithms of the equilibrium constant $(\lg K_f)$, entropies and molecular heat capacities (C_p^0) at 25^0 for gallium, indium and thallium compounds, mainly in the crystalline phase and partly in solution. As initial data were used those cited in references 5-11. General approximate formulas for all groups are given in table 1. Table 2 presents the calculated values of the formation heat of mixed halides of gallium, indium and thallium in crystalline

Card 1/3

Thermodynamic Properties of Calcium-,   SOV/79-29-5-3/75
Gallium-, Indium and Thallium Compounds

phase and of their solutions in HCl or water. The initial data
were gathered from the papers of references 5-7. Complementarily
the formation heats of the complex compounds $[Tl(H_2O)_4]Cl_2Br$
and $[Tl(H_2O)_4]ClBr_2$ were determined. The initial data are derived
from reference 11. The accuracy of the calculation depends on the
accuracy of the initial data. Further some thermodynamic
characteristic features of mixed calcium halides in crystalline
phase and partly in standard solution (HCl or H_2O) were calculated
according to the method described in reference 2 (Table 4).
Approximate general relationships with the determination of
thermodynamic properties of a number of crystal hydrates, ammoniates
and other calcium-containing compounds were derived from formula
(1) (Table 3). In tables 5 and 6 the calculated data for a large
group of compounds were compared with the data given in reference
5. They are found to be well consistent. The formulas given in
tables 2 and 3 for all compounds were published for the first
time and will be of use in practice. There are 6 tables and 11

Card 2/3   references, 5 of which are Soviet.

Thermodynamic Properties of Calcium-,
Gallium-, Indium and Thallium Compounds
SOV/79-29-5-3/75

ASSOCIATION: Voyenno-mekhanicheskiy institut (Military Mechanical Institute)

SUBMITTED: September 18, 1957

Card 3/3

5·(4)

AUTHOR: Maslov, P. G.   SOV/76-33-7-3/40

TITLE: Thermodynamic Properties of Sodium Compounds in Solid Phase. II

PERIODICAL: Zhurnal fizicheskoy khimii, 1959, Vol 33, Nr 7, pp 1461 - 1466
               (USSR)

ABSTRACT: Data on the thermodynamic properties of the hydrates of sodium
               salts in corresponding manuals are available only for some of
               these compounds, which are, however, important for a great
               variety of industrial applications. In previous papers (Refs 1-3),
               the author together with Yu. P. Maslov (Refs 4,5) devised meth-
               ods of determining the heat of formation and several other
               thermodynamic properties of many substances (among them also
               sodium compounds). In the present paper, the author analyzed
               the data of (Ref 6) by the above methods and obtained general

               approximate formulas for the heats of formation - ΔH_f^o, the free

               energy - ΔF_f^o, the logarithms of the constants of chemical equi-

               librium $\lg K_f$, the entropy S^o as well as for the specific heat

               C_p^o at 25° in solid (crystalline) state. The data were determined

Card 1/2

Thermodynamic Properties of Sodium Compounds in Solid   SOV/76-33-7-3/40
Phase.II

for 59 groups of hydrates and ammoniates of sodium compounds with about 800 substances. The above general formulas were represented for the following compounds: $NaF \cdot nH_2O$, $NaCl \cdot nH_2O$, $NaBr \cdot nH_2O$, $NaJ \cdot nH_2O$, $NaOH \cdot nH_2O$, $Na_2SO_3 \cdot nH_2O$, $Na_2SO_4 \cdot nH_2O$, $Na_2SiO_3 \cdot nH_2O$, $Na_2S \cdot nH_2O$, $Na_2Se \cdot nH_2O$, $NaHSO_4 \cdot nH_2O$, $NaHS \cdot nH_2O$, $Na_3PO_4 \cdot nH_2O$, $NaH_3P_2O_7 \cdot nH_2O$, $Na_2S_2O_6 \cdot nH_2O$, and $Na_2S_2O_3 \cdot nH_2O$, which may also be used for calculating the above values of other compounds of this kind. The calculation results (Tables 1-3) are in good agreement with the data of (Ref 6). Assuming that the values of (Ref 6) are exact, the calculation error is, according to the above equations, 0.2 - 1% (rarely 1 - 9%). There are 3 tables and 6 references, 5 of which are Soviet.

Card 2/2

5 (4)

AUTHORS: Maslov, P. G., Maslov, Yu. P. (Leningrad) SOV/76-33-8-2/39

TITLE: Thermodynamic Characteristics of Crystalline Compounds Containing
                Lithium. III

ABSTRACT: General approximation equations for the evaluation of the heat of
                formation (HF) and some other thermodynamic properties of
                crystalline compounds containing lithium were obtained for 25°C
                by means of the methods by P. G. Maslov (Refs 3, 5) from the
                corresponding data of the manual by T. D. Rossini et al (Ref 6).
                The calculation data, based on the principle of additivity, are
                given (Tables 1, 2) as well as the values obtained for (HF) -
                ΔH_f^O, the free energy - ΔF_f^O, the logarithms of the constants of
                chemical equilibrium log K_f, of the entropy S^O, and of the molar
                specific heat C_p^O for some crystal hydrates and ammoniates of the
                lithium compounds and other groups of compounds in the solid phase
                at 25°C (Tables 3, 4). A comparison with the data obtained from
                (Ref 6) shows a good agreement. The accuracy of the equations
                mentioned is sufficient for preliminary technological calculation
Card 1/2

Thermodynamic Characteristics of Crystalline Compounds   SOV/76-33-8-2/39
Containing Lithium. III

and is, on an average 0.2-1 %; in some individual cases 1-10 %.
There are 4 tables and 6 references, 5 of which are Soviet.

Card 2/2

5(4)

AUTHOR: Maslov, P. G.

TITLE: Thermodynamic Properties of the Halides of Cadmium Crystal
             Hydrates and Ammonates. IV

PERIODICAL: Zhurnal fizicheskoy khimii, 1959, Vol 33, Nr 9, pp 1951-1953
             (USSR)

ABSTRACT: As the knowledge of cadmium properties and its compounds is
             important for different technical branches, approximation
             formulas are deduced for the determination of the enthalpies
             ΔH^c_f, pertly for the determination of the free energy ΔZ^o_f, for
             the determination of the logarithms of the constants of
             chemical equilibrium $\lg K_f$, the entropy S^o and the specific
             heat C^o_p for halides, Cd-crystal hydrates and ammonates in
             solid phase at $25^o C$ (Table 1). The calculations are due to the
             methods (Refs 1,3-6). The above mentioned thermodynamical
             values were calculated by means of formulas as obtained by
             methods (Refs 5,6) for mixed cadmium halides (Table 2). The com-
             parison of the amounts for some compounds with those listed in
             the handbook by F. D. Rossini (Ref. 7), shows that the limit of

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SOV/76-33-9-10/37

Thermodynamic Properties of the Halides of Cadmium Crystal Hydrates and
Ammonates. IV

error of calculation equations applied amounts to about
0.5-1% and only for certain cases to 1-9%. There are 2 tables
and 7 references, 6 of which are Soviet.

Card 2/2

5.3300, 5.4700

77514
SOV/80-33-1-23/49

AUTHORS: Maslov, P. G., Maslov, Yu. P.

TITLE: Some Approximate Formulas for the Determination of Heat of Combustion and Heat of Formation of Gaseous Alkadienes

PERIODICAL: Zhurnal prikladnoy khimii, 1960, Vol 33, Nr 1, pp 134-140 (USSR)

ABSTRACT: Thermodynamic and other properties of chemical compounds can be expressed by the equation

$$A = a_1 + a_2 \cdot z \quad (\text{at } z \geqslant 4) \qquad (1)$$

where a_1 is an increment identical for the whole given homologous series; a_2 is the part of the characteristic A corresponding to the methyl group CH_2 in the linear chain C-C-C-...; z is the number

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Some Approximate Formulas for the
Determination of Heat of Combustion
and Heat of Formation of Gaseous
Alkadienes

77514
SOV/80-33-1-23/49

of CH_2-groups or C-atoms in this chain (P.G. Maslov, ZhFKh., 1952, Vol 26, p 1311; ibid., 1953, Vol 27, p 509). In the present study the authors established general formulas of type (1) for the determination of the heat of combustion and heat of formation of gaseous alkadienes at 25° C. The alkadienes were separated into groups having similar molecular structures, and the following formulas were suggested for the determination of the heat of combustion at 25° C under constant pressure: for 1-cis-3-alkadienes:

$$-\Delta Hc^o = (-24.31 + 157.44z) \; Cal/mole$$

for o-trans-3-alkadienes:

$$-\Delta Hc^o = (-25.24 + 157.44z) \; Cal/mole$$

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Some Approximate Formulas for the
Determination of Heat of Combustion
and Heat of Formation of Gaseous
Alkadienes

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SOV/80-33-1-23/49

for 2 methyl-1-cis-3-alkadienes:

$$-\Delta Hc^0 = (130.16 + 157.44z)\,Cal/mole$$

and so on. The above can be expressed by a general
formula for alkadienes:

$$-\Delta Hc^{\circ}_{gas} = -\left[24.31 - 15.42k_1 - 6k_2 + 0.938\sin\frac{\varphi}{2} - \right.$$
$$\left. - 154.47m_1 + 155.7m_2 + 1.63(\sigma-1)\right] + 157.44z \quad (at \quad z \geqslant 4), \qquad (2)$$

where k_1 is the number of C=C-bonds having a common
C-atom; k_2 is the number of C=C—bonds separated by
2 or more C-C-bonds in the main carbon chain of the
alkadiene (e.g., in 1,2-alkadienes $k_2 = 0$, $k_1 = 1$;

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Some Approximate Formulas for the
Determination of Heat of Combustion
and Heat of Formation of Gaseous
Alkadienes

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SOV/80-33-1-23/49

in 1,5-alkadienes $k_1 = 0$, $k_2 = 1$; etc); φ is the
angle of rotation of C=C-bonds from the original cis-
into trans- or trans-trans-position (it is assumed
that this angle is 0 in cis- or cis-cis-configurations
and is equal to π in cis-trans-trans- or trans-
trans-configurations); δ is the number of rotations
of C=C-bonds around the axis passing through the
bond=C-C=, from cis- or cis-cis-position into trans-,
cis-trans-, or trans-trans-position (e.g., in 1-trans-
3-alkadienes, $\delta = 1$ and $\varphi = \pi$; in 2-methyl-trans-
2-trans-4 alkadienes, $\delta = 2$, $\varphi = \pi$); m_1 is the
number of methyl groups in the molecule which re-
placed H-atoms at the second and last-but-one
C-atoms in the main alkadiene chain, and which
took part in the formation of C=C-bonds; m_2
is the number of methyl groups which replaced H-atoms

Card 4/7

Some Approximate Formulas for the
Determination of Heat of Combustion
and Heat of Formation of Gaseou_
Alkadienes

77514
SOV/80-33-1-23/49

belonging to the remaining C-atoms of the carbon
chain; σ is the smallest ordinal number of the
C-atom with the first C=C-bond; z is the number
of C-atoms in the unbranched alkadiene (e.g. z = 5
in all pentadienes). The heat of combustion in Eq.
2 is expressed in Cal/mole; the equation is valid for
alkadienes with $z \geqslant 4$, and gives only approximations
with $z \leqslant 4$. The heat of formation of gaseous alkadienes
at 25° C from the elements can be expressed similarly
by the equation

$$-\Delta H^{\circ}\ \textit{form. (el.)} = -\left[44.02 - 15.42 \cdot k_1 - 6k_2 - 0.936 \sin \frac{\varphi}{2} - \right.$$

$$\left. - 7.9 m_1 - 0.66 m_3 - 1.63\ (\sigma - 1) \right] + 4.93 z \quad (\textit{nr}\ z \geqslant 4) \qquad (3)$$

Card 5/7

and the heat of formation from atoms is correspondingly

Some Approximate Formulas for the
Determination of Heat of Combustion
and Heat of Formation of Gaseous
Alkadienes

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SOV/80-33-1-23/49

$$-\Delta H^\circ_{FORM}(AB)_a - \left[\, 148.39 - 14.42k_1 + 6k_2 - 0.935\sin\frac{\varphi}{2} - \right.$$

$$\left. - 238.44m_1 - 237.22m_2 - 1.63\,(\sigma - 1)\,\right] + 235\,5z \;\; (AT \; z \geqslant 4). \tag{4}$$

The values obtained from Eq. 2-4 are approximations,
which are close enough, however, to the best ex-
perimental data to serve in technological calculations
The errors do not exceed 1 to 1.5%. Comparative
tables of calculated and experimental heats of
combustions and heats of formations of numerous
alkadienes are given. There are 2 tables; and 8
references, 2 U.S., 6 Soviet. The U.S. references
are: J. Research Natl. Bur. of Standards, 1951, Vol
46, p 106; F. D. Rossini, K. S. Pitzer, R. L. Arnett,
R. M. Braun, G. C. Pimentel, Selected Values of
Physical and Thermodynamic Properties of Hydrocarbons

Card 6/7

Some Approximate Formulas for the
Determination of Heat of Combustion
and Heat of Formation of Gaseous
Alkadienes

77514
SOV/80-33-1-23/49

and Related Compounds, Publ. A. P. I., Pittsburgh, Pa.,
1953, p 458.

SUBMITTED: May 10, 1956; resubmitted, 1959.

Card 7/7

S/020/60/132/05/50/069
B011/B002

AUTHOR: Maslov, P. G.

TITLE: Some Physical Characteristics of the Alkyl Derivatives
              of Benzene

PERIODICAL: Doklady Akademii nauk SSSR, 1960, Vol. 132, No. 5,
              pp. 1156-1159

TEXT: The author used theoretical and semiempirical methods for the
investigation under review (Refs. 3-5). He shows the advantages of the
additive and additive-statistical methods. On the basis of such methods,
the author used approximate formulas for determining a number of charac-
teristics of various alkyl derivatives of benzene. It was found that the
critical parameters: pressure p_{cr}, volume V_{cr}, and density d_{cr} of
benzene derivatives containing up to four substituting methyl-, ethyl-,
propyl-, isopropyl-, or other groups, can be estimated by formulas (1),
(2), and (3). The reciprocal value of the critical compressibility coef-
ficient is determined from relation (4). In a similar way, the critical
temperature t_{cr} for the said derivatives with up to four substituting

Card 1/2

Some Physical Characteristics of the   S/020/60/132/05/50/069
Alkyl Derivatives of Benzene   B011/B002

radicals can be estimated by the general formula (5). The author then
deals with the methods used to determine the reciprocal value of the
pressure coefficient of temperature (6), the refractive indices for the
sodium line at $20^{\circ}C$ (7), and the boiling points at 760 mm (8). The data
of Ref. 1 served as the initial formulas. The values of some properties,
as estimated on the strength of the above formulas, are compared with
those from other sources in Tables 1 and 2, and a good agreement is
found. The accuracy of these formulas decreases with rising number of
substituents. Their average error fluctuates between 1 and 4%. They are
valid only for benzene derivatives with a maximum of four substituents.
There are 2 tables and 9 references: 8 Soviet and 1 American.

ASSOCIATION: Leningradskiy voyenno-mekhanicheskiy institut (Leningrad
              Military Mechanical Institute)

PRESENTED: February 15, 1960, by A. V. Topchiyev, Academician

SUBMITTED: September 4, 1959

Card 2/2

MASLOV, P.G.

Heats of formation of potassium compounds. Zhur. neorg. kh... 5
no.8:1669-1675 Ag '60.   (MIRA 13:9)

1. Leningradskiy voyenno-mekhanicheskiy institut, kafedra
fiziki.
      (Potassium compounds)   (Heat of formation)

37768
S/661/61/000/006/058/031
D267/D502

24 5300
5.3700
11.2219

AUTHORS: Maslov, P. G. and Maslov, Yu. P.

TITLE: A new statistical method of calculating thermodynamic
           properties

SOURCE: Khimiya i prakticheskoye primeneniye kremneorganicheskikh
           soyedineniy; trudy konferentsii, no. 6: Doklady, diskus-
           sii, resheniye. II Vses. konfer. po khimii i prakt. prim.
           kremneorg. soyed., Len. 1958. Leningrad, Izd-vo AN SSSR,
           1961, 240-258

TEXT: The authors present a new generalized version of the sta-
tistical method, based on the results of their earlier research
work. The new method differs from the conventional methods by a
great simplicity of operation, associated with great accuracy,
close to that of the widely known methods, which, however, necessi-
tate knowledge of vibrations spectra, electronic levels and of the
nature of stopped rotations. The molecular characteristics (molecu-
lar weights, principal moments of inertia and symmetry numbers)

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A new statistical method...

S/661/61/000/006/058/081
D267/D302

are required only for calculating the properties of the type of
entropy and of the $\bar{Q}^x$-potential. Properties such as heat capacity,
heat content, heats of combustion and formation, physico-chemical
characteristics of vaporization, ionization potentials, energies
of dissociation, boiling points and critical parameters are ob-
tained directly from formulas. The method can be applied to all
compounds, in particular to organosilicon, organo-metallic and in-
organic compounds. The calculated results are in very good agree-
ment with the results of measurements, and with calculations made
by other authors. Three numerical examples are given. There are 5
tables and 28 references: 21 Soviet-bloc and 7 non-Soviet-bloc. The
4 most recent references to the English-language publications read
as follows: A. S. Friedman and L. Haar, J. Chem. Phys., 73, 5259,
(1954); E. V. Ivash, J. C. M. Li and K. S. Pitzer, J. Chem. Phys.,
23, 1814, (1955); C. M. Lia, James and K. S. Pitzer, J. Phys. Chem.,
60, 466, (1956); G. J. Janz and S. C. Whit, Jr., J. Chem. Phys.,
26, 1766, (1957).

Card 2/2

15.8170
5.4800

37769
S/661/61/000/006/059/081
D267/D302

AUTHORS: Maslov, P. G. and Klochikhin, A. A.

TITLE: Thermodynamic properties of fluorochlorosilanes $SiFCl_3$, SiF_2Cl_2, SiF_3Cl

SOURCE: Khimiya i prakticheskoye primeneniye kremneorganiches-kikh soyedineniy; trudy konferentsii, no. 6: Doklady, diskussii, resheniye. II Vses. konfer. po khimii i prakt. prim. kremneorg. soyed., Len. 1958. Leningrad, Izd-vo, AN SSSR, 1961, 259-265

TEXT: In view of the growing interest in the physico-chemical (especially the thermodynamic) properties of silane derivatives which cannot be easily determined, various additive and additive-statistical methods appear to be useful. The authors recommend for this purpose a new additive-statistical method developed by one of them (Ref. 9: ZhFKh, 32, 1715, (1958)); (Ref. 10: Optika i spektr., 3, 38, (1957)) and characterized by very simple formulas associated

Card 1/3

Thermodynamic properties of ...

with the same accuracy as found in purely statistical methods. The following magnitudes were calculated in this paper: The potential $\phi^* = (F^0 - E_0^0)_T$, the entropy S^0, the enthalpy $H_T^0 - H_0^0$, the total enthalpy I_T^0, the logarithms of chemical equilibrium constants (log K_p) for the processes of formation of gaseous compounds $SiFCl_3$, SiF_2Cl_2 and SiF_3Cl at p = 1 atm. from atoms in a wide temperature interval (298.16 - 2500°K), and their energy of dissociation D_0. Sources of basic data are indicated. Certain assumptions have been made. The results of calculations are presented in tabular form; their accuracy is of the order of 0.1 - 1.5%. No corresponding experimental results are available. There are 3 tables and 24 references: 11 Soviet-bloc and 13 non-Soviet-bloc. The 4 most recent references to the English-language publications read as follows: H. Murata, K. Kawai, J. Chem. Phys., 23, 2451, (1955); A. P. Altschuller, J. Chem. Phys., 23, 761, (1955); D. W. Mayo, H. E. Opitz,

Card 2/3

Thermodynamic properties of ...   S/661/61/000/006/059/081
D267/D302

and J. S. Peake, J. Chem. Phys., 23, 1344, (1955); M. J. Hawkins
and W. M. Kent, J. Chem. Phys., 24, 385, (1956).

ASSOCIATION: Leningradskiy mekhanicheskiy institut (Leningrad In-
stitute of Mechanics)

Card 3/3

MASLOV, P.G. (Leningrad); MASLOV, Yu.P. (Leningrad)

Method of computing thermodynamic properties without the knowledge
of electronic and vibrational spectra. Zhur. fiz. khim. 35 no.1:
164-175 Ja '61.   (MIRA 14:2)
                        (Thermodynamics)

16.6200

5.4300

2634
S/076/61/035/007/015/019
B132/B220

AUTHOR: Maslov, P. G.

TITLE: Methods of investigating the reactivity of radicals

PERIODICAL: Zhurnal fizicheskoy khimii, v. 35, no. 7, 1961, 1551-1557

TEXT: A new statistical method of studying some problems of chemical
kinetics and reactivity is described. It permits to calculate the heat
content, the dissociation and ionization energies, and some other
properties of all i-th members of a selected family of compounds from the
analogous properties of the j-th members by using the equation:

$$B_i = (\frac{1}{s}) \sum_j d_j B_j \quad (1).$$

B is the quantity of the property studied, s the maximum

valence of group A, which is the same for all members of the family
selected, d_j the numerical factor of B_j. Moreover, the reaction heat q

equals the difference of the formation energy D' of the new bond in the
reaction products and the rupture energy D of the bond in the initial
substance, or the difference of activation energy of the endothermic (E)

Card 1/5

26344
s/076/61/035/007/015/019

Methods of investigating ...   B132/B220

and the reversible exothermic reaction $(\mathcal{E}_o)$: $q = D' - D = \mathcal{E} - \mathcal{E}_o$ (2). The
rupture (dissociation) energy is determined from Eq. (1). The equation
$q_i = (\frac{1}{s}) \sum_j \mathcal{J}_j q_j$ (3) holds. Therefrom, it results that the activation energies
can be calculated from Eq. (1). This follows from the relation $\ln(Z/k) = -\mathcal{E}/RT$ (4) determining the collision effectivity Z/k. Thus: $\ln(Z/k)_i = -(\frac{1}{s}) \sum_j \mathcal{J}_j \ln(Z/k)_j$ (5). It may be regarded as proved that Eq. (1) and the

method by P. G. Maslov and Yu. P. Maslov (Ref. 9: Optika i spektroskopiya,
7, 355, 1955; Ref. 10: Zh. fiz. khimii, 32, 1715, 1958; Ref. 11: P. G.
Maslov, Optika i spektroskopiya, 7, 355, 1959) are suitable for determining
the thermodynamic properties of radicals, the rupture energies of bonds,
the activation energies, heat effects, and reaction rate constants. This
is illustrated by a discussion of the determination of the rupture energy
of the C-Cl bond in the molecules $CHCl_3$, CH_2Cl_2, C_2H_5Cl, and iso-C_3H_7Cl
from the corresponding values 83.5, 67.9, and 75 kcal/mole for the
molecules CH_3Cl, CCl_4, and $C(CH_3)_3Cl$. Furthermore, activation energies

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S/076/61/035/007/015/019
B132/B220

Methods of investigating ...

and heat effects of the substitution reactions $Na+RCl \longrightarrow NaCl+R$ were determined. The initial values for calculating the bond rupture energies are given in Table 1; the values obtained by the author are marked with two asterisks. For determining any property Δ of the members of a family of the type $BR_s^{(1)}$, which only contain functional groups $R^{(1)}$, a general relation of the form

$$\Delta_{(cp)\,[BR_s^{(1)}]} = \frac{1}{t}\sum_{j=1}^{t}\left[\frac{s}{q_j}\Delta_{\left[BR_{q_j}^{(1)}\prod_{i=2}^{l}{}^{'}R_{a_i}^{(i)}\right]} - \frac{1}{q_j}\sum_{i=2}^{l}a_i\Delta_{[BR_s^{(1)}]}\right]_j \,, \qquad (7)$$

may be derived from the values of the remaining members $BR_{q_j}^{(1)}\prod_{i=2}^{l}R_{a_i}^{(i)}$ containing $R^{(1)}$; the subscript (cp) denotes that it is a mean value. $BR_s^{(i)}$ are the completely substituted members of the family of cognate compounds containing only the group $R^{(i)}$; t is the number of compounds containing the group $R^{(1)}$ and used for determining $D_{BR_s}^{(i)}$. There are. Card 3/5

26344

S/076/61/035/007/015/019
B132/B220

Methods of investigating...

7 tables and 15 references: 13 Soviet-bloc and 2 non-Soviet-bloc.

SUBMITTED: November 20, 1959

Table 1. Data on bond rupture or dissociation energies, taken for
initial values, correct if the author's method is used, in kcal/mole.
Legend: (A) Compound and point of rupture of the bond R - X; (B) author's
data; (C) experimental value.

Card 4/5

5.4100

166200

26276
S/064/61/000/008/003/003
B103/B208

AUTHOR: Maslov, P. G.

TITLE: New methods in the study of physico-chemical properties
            of matter

PERIODICAL: Khimicheskaya promyshlennost', no. 8, 1961, 21-26

TEXT: The absence of reliable physico-chemical characteristics renders the
calculation of many technological processes impossible. These properties
especially the thermodynamic ones cannot be determined by experimental means
alone, which is, however, not considered necessary by the author. He
suggests for this purpose an additive-statistical method of calculation
which is suitable for the examination of any substance, particularly the
physico-chemical characteristics of families of complicated compounds may
thus be determined simply and exactly. The knowledge of vibrational spectra
and of other molecular data is not necessary. In order to determine the
value of a certain property of all members, it will be sufficient to know
the respective property of only some simple representatives of this family.
The initial supposition of the method mentioned is a peculiar additivity

Card 1/6

New methods in the study ...

26276
S/064/61/000/008/003/003
B103/B208

(according to P. G. Maslov, (Uspekhi khimii, 25, 1069 (1956); I. N. Godnev
(Ref. 18: Vychisleniye termodinamicheskikh funktsiy po molekulyarnym dannym
(Calculation of thermodynamic functions from molecular data) GITTL, 1956))
of the electron and vibrational spectra of the families of related compounds
according to P. G. and Yu. P. Maslov (Ref. 40: Optika i spektr, 3, 38
(1957); 7, 355 (1959)). The application of the author's method is exempli-
fied by the halide family of the $AX_{n_1}^{(1)}X_{n_2}^{(2)}....X_{n_t}^{(t)}$ type, where $X^{(i)}$

[Abstracter's note: (1) or (i) is a printing error] are halogens, hydrogen,
or other structural groups; A is an atom or atom group which is common to
all members of the family; in the case of halogen derivatives of methane,
ethane, silane $A = C$, C_2 etc. The author assumes that the property B
concerned is known for the simplest j members AX'_n, $AX''_n....AX^{(t)}$, and the
absolute values of B for the remaining i representatives of the same family
are to be determined. The value B is then obtained in the general case
under the same conditions from the following relation:

$$B_i = 1/n \sum_j n_j B_j - \Delta_M - \Delta_D + \Delta_\sigma - \Delta_\gamma - \Delta_\alpha - \Delta' + B_{def.rot:}, \text{where } n = n_1 + n_2 + ...n_j$$

Card 2/6

New methods in the study ...

is the valence of the coordinating atom or of the atom group A, n_j is the number of atoms of the $X^{(1)}$ type in the molecules of the compound, Δ_M is the correction for the change in molecular weight, M. $\Delta M \approx 3R/2n$ $\left(\sum n_j \ln M_j - n \ln m_i\right)$ (2). Δ_D is the correction for the change of the main moments of inertia. $D = I_A \cdot I_B \cdot I_C$; $\Delta_D = R/2n\left(\sum_j n_j \ln D_j - n \ln D_i\right)$ (3). Δ_k is the change of the number of symmetry of the molecules $(k = \sigma)$, of the electron sum $(k = \rho)$, or of the spin variable $(k = \phi)$. Δ_k (4), Δ' and b_o (6) see in the figure, where k = Boltzmann's constant, T - temperature in ^{o}K, and h = Planck's constant. The correction $B_{def.rot.}$ (def.rot. - deferred rotations) is determined either by the usual way according to K. S. Pitzer, W. P. Gwinn. (Ref. 18; Ref. 20: J. Chem. Phys., 10, 428 (1942)) or in the first approximation according to the expression: $B_{def.rot.} = 1/n\sum_j n_j B_{def.rot.j}$ (7). In the

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S/064/61/000/008/003/003
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latter case, the correction automatically forms a constituent of the sum (1) and need not be determined in particular. The author proved in Ref. 40 that the corrections Δ' and $\Delta\rho$ are practically equal to zero for $T > 50°K$. At sufficiently high T, also Δ_{ν} equals zero. Hence, only the corrections Δ_{M}, Δ_{D} and Δ_{σ} are calculated for the gas phase. They are only necessary to determine the entropy S^o, the potential $\phi^* = -(F^o - E_o^o)/T$, and the logarithm of the constant of chemical equilibrium $\log K_{eq}$. When calculating heat capacities, enthalpy, total enthalpy, heats of combustion and formation, as well as the thermodynamic characteristics of the phase inversions, corrections (2) - (5) are not calculated, as in this case the properties B_i are directly determined

from the expression $B_i = 1/n \sum_j n_j B_j$ (1^I). All values of the thermodynamic

properties are determined from (1^I) for the solid and the liquid phase of

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compounds with similar lattice structures without any corrections. If not only the simplest AX_n^i but also complex $AX'X''_{q\ r}$ are used as initial compounds, (1^{II}) is applied:

$$B_1 = 1/S_0 \sum_j d_j B_j - \Delta_M - \Delta_D - \cdots - \Delta_2 - \Delta_i - \Delta' + B_{def.rot.} \ (1^{II}), \text{ where } S_0 = \sum_j d_j, \ d_j$$

is the number that indicates how many times B_j is to be taken as a summand for the j-th initial compound. Calculations revealed that the author's method is also suitable to determine the molecular refraction R_D, the coefficients of surface tension, critical temperature, viscosities, parachors, refrachors, thermochemical radii, dissolution energy, temperature of evaporation, and other quantities. This applicability is not yet theoretically substantiated, but is still an empirical fact. The author gives some examples of calculation. He concludes therefrom that his method provides the values of the above-mentioned properties with sufficient precision, in a simple way and within a short time. Besides, the frequencies of the vibrational spectra,

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their intensities, density, refractive indices, and other characteristics may thus be determined. This method permits the solution of many practical problems by scientists and plant staff. There are 5 tables, and 44 references: 40 Soviet-bloc and 4 non-Soviet-bloc. The references to English-language publications read as follows: C. J. Janz, S. C. Wait, Jr., Chem. Phys., 26, 1766 (1957); F. D. Rossini et al. Selected Values of Chemical Thermodynamic Properties, Circ. of the Natl. Bur. of Standards, Washington, 1952, P. 500.

$$\Delta_k = \frac{R}{n}\left(\sum_j n_j \ln K_j - n \ln K_i\right) \qquad (4)$$

$$\Delta' = \frac{R}{S_0}\left\{\sum_j n_j\left[\ln(1+\delta_0) + \frac{\beta_0}{4(I_B \cdot I_C)^{0.5}}\right]_j - \right.$$

$$\left. - n\left[\ln(1+\delta_0) + \frac{\beta_0}{4(I_B \cdot I_C)^{0.5}}\right]_i\right\} \qquad (5)$$

$$\beta_0 = h^2/8\pi^2 kT$$

$$\delta_q = \frac{\beta_0}{12(I_B \cdot I_C)^{0.5}}\left[1 - \frac{I_A}{(I_B \cdot I_C)^{0.5}}\right] \qquad (6)$$

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